LARGE EDDY SIMULATIONS OF BUOYANT PLUMES

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ABSTRACT

An approach to the study of gas phase combustion and convection processes in fires using a combination of mathematical analysis and computer simulation is presented. It seeks to solve the governing equations directly (if approximately) by decomposing the fire into a large scale convective and radiative transport problem coupled to a small scale model of combustion and radiative emission. The combustion model assumes that all of the thermodynamic properties of the fluid are tied to the local mixture fraction, which is convected by the large scale motion, which in turn is driven by the heat released by the combustion processes. The large scale flow is studied using finite difference techniques to solve large eddy simulations of the Navier-Stokes equations. As a first test of the numerical approach a buoyant helium plume is simulated and results compared to a companion laboratory experiment.

INTRODUCTION

The difficulties associated with analyses of fire phenomena originate with the fact that the active combustion zone of a fire plays two distinct roles which encompass widely different length and time scales. The combustion zone is the region where the local mixing of gasified fuel and air produces the chemical energy release and radiant energy emission that sustains the fire. These processes occur on length scales ranging from a fraction of a millimeter to a few centimeters. At the same time, the combustion zone is a source of buoyancy which induces large scale mixing of air and combustion products, forming a plume which can persist as an organized structure over length scales ranging from a few meters to tens of kilometers, depending on the scenario of interest. The plume in turn, acts as a giant pump that induces a flow pattern throughout the entire structure enclosing an indoor fire. Equally important, the interaction of the large scale mixing and small scale combustion processes creates a combustion zone that is not necessarily small compared with the plume that it generates. Finally, the radiative transport from the entire combustion zone back to the condensed phase fuel surface provides the feedback needed to supply the fire with the fuel required to maintain itself.

Much of the work in fire research concerns the movement of smoke and hot gases in an enclosure. Depending on the scope of the particular scenario, the fire itself is described in relatively simple terms as a source of heat and combustion products [1]. The reason for this is that the fire itself usually occupies a very small fraction of the flow domain; and there is simply not enough spatial resolution to describe fluid motion on length scales at which combustion takes place. Conventional field models using k-ε representations of turbulence often include an empirical description of the combustion processes, but this description relies heavily on the level of turbulence prescribed by the user through the choice of parameters. The approach outlined below, by contrast, seeks approximate solutions to the governing equations directly, by considering combustion, convection, and thermal radiation in parallel, allowing each to evolve separately on its own length and time scale. The complexity of the combustion model which is implemented depends on the spatial and temporal resolution which can be provided by the solution of the Navier-Stokes equations without any empirical turbulence model. Present computational resources allow for two-dimensional simulations with Reynolds numbers approaching 10^5, and three-dimensional calculations approaching 10^4. In the present work, a few 2D, axisymmetric plume simulations will be presented. Simulations in 3D are presently underway, as is the implementation of a soot and radiation model. Before these more elaborate additions are made, however, we seek confirmation that the hydrodynamic model adequately describes the flow field. As a first test of the hydrodynamic model a buoyant helium plume was simulated and the results compared to those from laboratory experiments. The approach taken for both the combustion and isothermal scenarios is presented next, followed by helium plume results.

NUMERICAL MODEL

Following the analysis of Rehm and Baum [2], we assume that the flow velocity is much less than the sound speed; the temperature and density variations are large, but the pressure variations are small. The gases are assumed to be ideal and variable transport properties are allowed. Under these assumptions the equation of state and conservation equations for momentum and total mass are

$$p_o = \rho R T \sum_i \frac{Y_i}{W_i}, \tag{1}$$

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$$\frac{\partial}{\partial t}\rho\underline{u} + \nabla \cdot (\rho\underline{u}\underline{u}) + \nabla p - (\rho - \rho_\infty)\underline{g} = \nabla \cdot \underline{\underline{\sigma}}, \tag{2}$$

$$\frac{\partial}{\partial t}\rho + \nabla \cdot \rho\underline{u} = 0. \tag{3}$$

Here p_0 is the spatially independent background pressure, p the perturbation of pressure from ambient, R the gas constant equal to the difference of the specific heats $R = c_p - c_v$ which are assumed to be constant, ρ the local density, ρ_∞ the ambient air density, $\underline{u}$ the velocity vector, $\underline{g}$ the gravity vector and $\underline{\underline{\sigma}}$ the standard viscosity stress tensor.

In addition to equations (1) - (3) the equations governing the conservation of energy and species mass fractions are required. The energy equation expressed in terms of the temperature is

$$\rho c_p\left(\frac{\partial T}{\partial t} + \underline{u} \cdot \nabla T\right) - \frac{dp_o}{dt} = \nabla \cdot (\rho k \nabla T) + \dot{q}\,, \tag{4}$$

where T is the temperature, k the thermal conductivity, $\dot{q}$ the heat release rate due to combustion. With the assumption of constant average molecular weight, $\overline{W} = \sum Y_i / W_i$, an equation for the background pressure can be derived from equations (1) and (4):

$$\left(1 - \frac{R\overline{W}}{c_p}\right)\frac{d}{dt}p_o + p_o(\nabla \cdot \underline{u}) = \frac{R\overline{W}}{c_p}[\dot{q} + \nabla \cdot (\rho k \nabla T)]\,. \tag{5}$$

For the case of an unenclosed domain $dp_o/dt = 0$ and $p_o = 1$.

With the assumption of a unity Lewis number and appropriate boundary conditions the temperature can be related to a mixture fraction variable and a species mass fraction. The mixture fraction, $Z(\underline{x}, t)$, is the solution to equation

$$\rho\left(\frac{\partial Z}{\partial t} + \underline{u} \cdot \nabla Z\right) = \nabla \cdot (\rho D \nabla Z), \tag{6}$$

where D is the mass diffusivity. The direct calculation of the combustion processes would require the solution of the equations of motion including the mixture fraction down to length scales at which the diffusive processes dominate the convective motion. This is not feasible at present, since the active combustion zone of a fire is usually only a small fraction of the space that must be included in any simulation. As a first step in the attempt to include realistic chemical heat release, the combustion process is idealized as a single global reaction which proceeds at an effectively infinite rate whenever the reactants come into contact [3]. With this assumption the species mass fraction and, therefore, temperature (density) are functions of the mixture fraction. An empirically based functional relationship between mixture fraction and density can be extracted from experiments [3]. With the relationship between density and mixture fraction known the complete combustion problem is governed by Eqs. (1), (2), (5) and (6).

Before implementing the combustion model discussed above the numerical approach was tested by simulating a buoyant helium plume. Since the helium/air density ratio (1/7) is similar to that found in fires the helium plume is an appropriate test. Analogous laboratory experiments provided a data base against which to compare the results of the simulations. The governing equations are those for the isothermal mixing of helium and air in the low Mach number limit. The gases are assumed to be ideal and transport coefficients vary. The motion of the gas is governed by the conservation equations for momentum [Eq. (2)], total mass [Eq. (3)] and the helium mass fraction (Y):

$$\rho\left(\frac{\partial}{\partial t}Y + \underline{u} \cdot \nabla Y\right) = \nabla \cdot (\rho D \nabla Y), \tag{7}$$

where D is the binary mass diffusivity. The equation for the background pressure, analogous to Eq.(5), can be obtained from the equation of state and a linear combination of Eqs. (3) and (7):

$$\frac{d}{dt}p_o + p_o(\nabla \cdot \underline{u}) = RT\left(\frac{1}{w_H} - \frac{1}{w_A}\right)\nabla \cdot (\rho D \nabla Y), \tag{8}$$

where w_H and w_A are the molecular weights of helium and air, respectively.

RESULTS

The simplified equations above are nondimensionalized, written in cylindrical coordinates, and solved with a finite difference technique. All spatial derivatives are approximated by second-order accurate central differences on a grid which is uniform in the axial direction and stretched in the radial direction. The solution is advanced in time with a simple Runge-Kutta scheme or other predictor-corrector scheme. A projection method [4] is used to determine the pressure field. The

examples below are two-dimensional, axially-symmetric, but the methodology is suitable for two or three spatial dimensions and any coordinate system. The scenario of interest is pure helium exiting from a circular pipe at low velocities relative to the characteristic buoyant velocity. The range of Froude numbers covered is $0.0015 \leq Fr \leq 0.64$ ($Fr = U_0^2 / Dg$, where U_0 is varied and equals the exit velocity of the helium from the pipe, D=7.3cm is the pipe diameter and g is the acceleration of gravity). Thus, the motion of the plume is due to buoyancy. The space surrounding the pipe is closed. Simulations are begun by instantaneously rupturing an imaginary membrane covering the pipe opening.

The structure of the plume is governed by the periodic shedding of toroidal vortices. This shedding is seen as a series of pulsations whose frequency is inversely proportional to the square root of the orifice diameter. Figure 1 is a snapshot of the simulated and the experimental plume. Helium mass fraction is contoured for the simulation while the experimental contours are pixel values from a video recording of the water seeded helium plume. The formation of a vortex can be clearly seen in both cases. Cetegen and Ahmed [5] refined this correlation to show dependence of initial velocity. As a first check on the accuracy of the hydrodynamics, the frequency of the simulated plume pulsations was checked against experimental values. Figure 2 is a plot of the Stouhal number, $St = fD / U_0$, versus the inverse of the Froude number. Results from both the current experiment and that of Hamins *et al.* are included. The experimental data was well fit by power laws, each of which is plotted on the figure. The pulsation frequencies of the simulated plume can be seen to be in good agreement with the experiments.

There are three possible sources of vorticity: the baroclinic torque, buoyancy and viscosity (largely due to drag along solid surfaces). The pulsations are mainly due to the formation of toroidal vortices by the baroclinic torque at the base of the plume. This can be clearly seen in the numerical simulation by 'turning off' the baroclinic torque (not shown). Without the presence of the baroclinic torque the plume still pulsates, due to buoyancy generated vorticity, but at significantly higher frequencies.

The major physical approximation in the simulation is that the plume evolves in an axisymmetric manner. For a number of reasons, this assumption is expected to be less valid with increasing axial distance from the pipe outlet. Figure 3 shows the time averaged centerline velocity and helium mass fraction for the $Fr = 0.32$ case. As expected the disagreement between simulated and experimental values increases with axial distance. With increasing axial distance relatively less mixing occurred in the simulation, which results in a buoyancy induced axial velocity which is larger than the experimental values. Figure 1 also shows an increasing discrepancy with height between simulation and experiment. Some caution should be exercised when viewing Fig. 1 since the water vapor in the experiment undergoes evaporation and high Schmidt number diffusion. The calculations shown here were on a grid with 96 cells in the radial direction and 384 cells in the axial. This represents a modest calculation with approximately 2.5 hours of CPU time on an IBM/RISC 6000 workstation corresponding to 1sec of real time. A more realistic three-dimensional calculation at the same temporal and spatial resolution would require a prohibitively larger amount of CPU time (~ 1 week).

CONCLUSION

Axisymmetric simulations of a buoyancy driven helium plume were largely found to be in good agreement with experiments. Differences between the simulation and experiments increased with axial distance and were most likely due to three-dimensional effects. Assuming that further results for the nonreacting plume compare favorably with the experiments, combustion, soot production and radiation can then be added. The complexity of these additions will depend on the spatial and temporal resolution which can be achieved in the non-reacting case, which obviously depends on whether the simulation is two or three dimensional.

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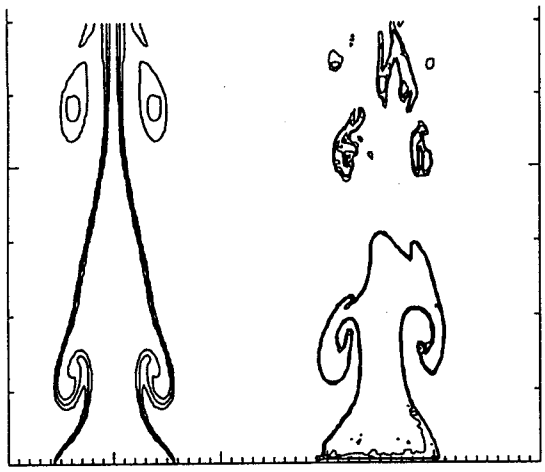


Figure 1 Snapshot of simulation (on the right) and the experiment. Contours correspond to helium mass fraction values in the simulation and pixel values from a video recording of the water seeded helium in the experiment.

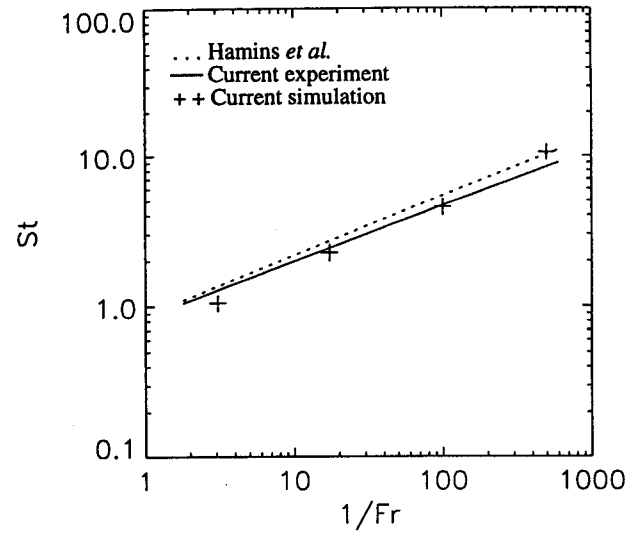
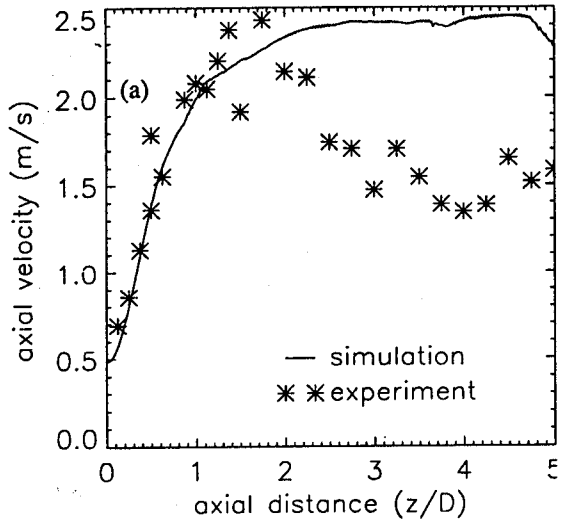


Figure 2 Strouhal number of plume pulsations, $St = fD/U_o$, versus $1/Fr = gD/U_o^2$. The experimental results of both the current study and that of Hamins *et al.* are shown along with results from the simulation.



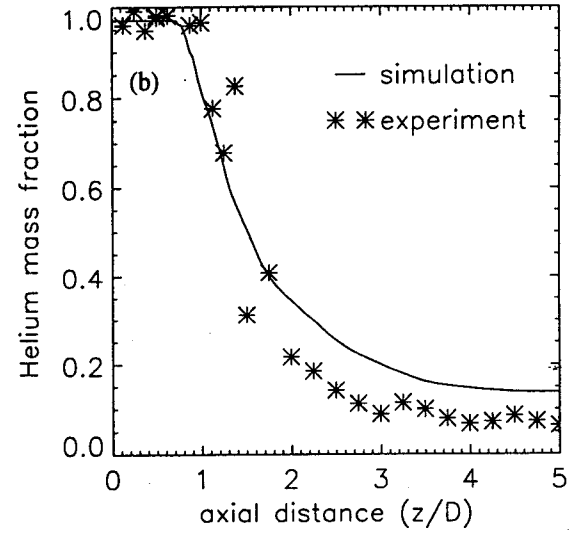


Figure 3 Time averaged centerline profiles of (a) the axial velocity and (b) the helium mass fraction. Both simulated and experimental results are shown for a Froude number, $Fr = U_o^2 / gD = 0.32$.